Computational design of carbon nanotube network materials and polymer matrix nanocomposites

Completed Technology Project (2016 - 2020)

Project Introduction

Carbon nanotube (CNT) network materials constitute a broad class of multifunctional materials that possess a unique combination of structural, mechanical and transport properties, making them attractive for various aerospace applications. The complexity of the hierarchical multiscale organization of the CNT materials, wide diversity of material structures and variability of physical properties present a challenge for theoretical evaluation of the structure-properties relationships and define the critical role the computational modeling can play in designing the advanced CNT materials. A team of researchers from the University of Virginia and University of Alabama will work on the development of a robust mesoscopic model capable of bridging the gap between the behavior and properties of nanoscale structural features of CNT-based materials revealed in atomistic simulations and the effective macroscopic properties defined by the collective behavior of multiple nanotubes and their interaction with a polymer matrix. The capabilities of the model will be demonstrated in analysis of the structural, mechanical, and transport properties of the CNT materials and nanocomposites. The results of the proposed study will facilitate the development of multifunctional low-density materials with unique combination of mechanical and transport properties tailored for aerospace applications.

Anticipated Benefits

This work includes development of a robust mesoscopic model capable of bridging the gap between the behavior and properties of nanoscale structural features of CNT-based materials revealed in atomistic simulations and the effective macroscopic properties defined by the collective behavior of multiple nanotubes and their interaction with a polymer matrix. The results of this study will facilitate the development of multifunctional low-density materials with unique combination of mechanical and transport properties tailored for aerospace applications.

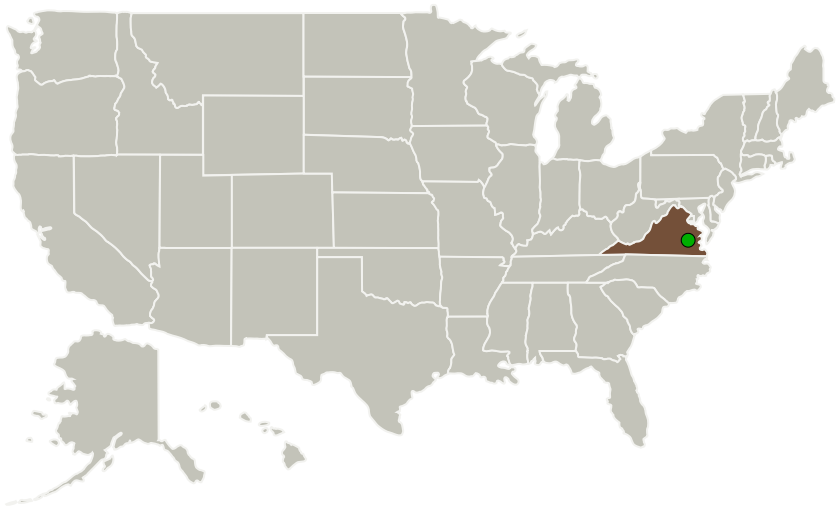
Computational design of carbon nanotube network materials and polymer matrix nanocomposites

Table of Contents

Computational design of carbon nanotube network materials and polymer matrix nanocomposites

Completed Technology Project (2016 - 2020)

Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
University of Virginia-Main Campus	Lead Organization	Academia	Charlottesville, Virginia
Langley Research Center(LaRC)	Supporting Organization	NASA Center	Hampton, Virginia

Primary U.S. Work Locations
Virginia

Project Website:

https://www.nasa.gov/strg#.VQb6T0jJzyE

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Organization:

University of Virginia-Main Campus

Responsible Program:

Space Technology Research Grants

Project Management

Program Director:

Claudia M Meyer

Program Manager:

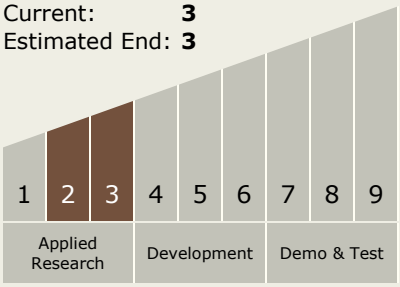
Hung D Nguyen

Principal Investigator:

Leonid V Zhigilei

Technology Maturity (TRL)

Start: **2**
Current: **3**
Estimated End: **3**



Computational design of carbon nanotube network materials and polymer matrix nanocomposites

Completed Technology Project (2016 - 2020)

Technology Areas

Primary:

- TX12 Materials, Structures, Mechanical Systems, and Manufacturing
  - TX12.1 Materials
    - TX12.1.1 Lightweight Structural Materials

Target Destination

Outside the Solar System